

CLAIMS

What Is Claimed Is:

- 1 1. A method comprising:
2 predicting a secondary structure of a protein;
3 superimposing the predicted secondary structure on a set of topomers;
4 refining the superimposed secondary structure; and
5 predicting a tertiary structure of a protein
- 1 2. The method of claim 1, wherein said secondary structure is a consensus
2 secondary structure prediction.
- 1 3. The method of claim 1, further comprising annealing the secondary structure by
2 energy minimization.
- 1 4. The method of claim 3, wherein said energy minimization is by a random
2 Monte Carlo method.
- 1 5. The method of claim 4, wherein the random Monte Carlo method uses random
2 moves from a log probability table.
- 1 6. The method of claim 3, wherein the random Monte Carlo method uses smart
2 moves.
- 1 7. The method of claim 1, wherein the secondary structure superimposed on a set
2 of topomers is refined by energy minimization.
- 1 8. The method of claim 7, wherein the secondary structure superimposed on a set
2 of topomers is refined using a molecular modeling program.
- 1 9. The method of claim 8, wherein the molecular modeling program is X-PLOR.
- 1 10. A method comprising:
2 predicting a secondary structure of a protein;
3 generating a three-dimensional representation of the predicted secondary structure;

4 optimizing the secondary structure by adjusting dihedral angles using smart moves; and
5 determining a three-dimensional protein structure by modeling the optimized secondary
6 structure on a topomer model.

1 11. The method of claim 10, wherein said secondary structure is a consensus
2 secondary structure prediction.

1 12. The method of claim 10, wherein optimization is performed using a random
2 Monte Carlo method.

1 13. The method of claim 12, wherein the random Monte Carlo method is used in
2 conjunction with a localized energy function.

1 14. The method of claim 10, wherein said three-dimensional structure model is
2 refined using simulated annealing.

1 15. A machine readable medium that provides instructions, which when executed
2 by a machine cause said machine to perform a method comprising:
3 predicting a secondary structure of protein;
4 superimposing the secondary structure on a topomer model; and
5 refining the topomer model.

1 16. A machine readable medium as in claim 15, wherein said secondary structure is
2 a consensus secondary structure prediction.

1 17. A machine readable medium as in claim 15, further comprising energy
2 minimization of the secondary structure prediction.

1 18. A machine readable medium as in claim 17, wherein said energy minimization
2 is by a random Monte Carlo method.

1 19. A machine readable medium as in claim 18, wherein random moves are selected
2 from a log probability table.

1 20. A machine readable medium as in claim 15, wherein the topomer model is
2 refined by topological entropy minimization.

1 21. A machine readable medium as in claim 20, wherein the topomer model is
2 refined by a molecular modeling program.

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